10. POLYMER CRYSTALLOGRAPHY

Drick, 1976). A posterior difference map revealed positions for ten H-atoms. The refinement was terminated at $R = 0.039$, $R_w = 0.036$.

The two Cu atoms lies on two different octahedral coordination sites. The $[\text{Cu(H}_2\text{O)}_4\text{OII}]^{2-}$ coordination polyhedron is a slightly distorted octahedron and the $[\text{Cu(CDTA)}]^2-$ has a more distorted octahedral geometry.

The two coordination polyhedra are linked by carboxylate bridges forming infinite zig-zag chains along $a$, with the plane of the zig-zag parallel to $(001)$.

10.3-1 INVESTIGATION ON THE $\beta \rightarrow \alpha$ POLYMORPHIC TRANSITION IN ISOTACTIC POLYPROPYLENE.

By D.Paukszta and J.Garbarczyk, Department of Chemistry, Technical University, Poznan, Poland.

In our previous works we had found, that less stable hexagonal $/\beta/$ polymorphic form /besides monoclinic-$/\alpha/$ of isotactic polypropylene is formed during crystallization from a melt in presence of a small amount of aromatic compounds having specific crystal structure /Garbarczyk, Paukszta, Polymer 1981,22,562/. Energetic calculations show that experimental observation of hexagonal form is made possible owing to retardation polymorphic $\beta \rightarrow \alpha$ transition /Garbarczyk, Die Makrom. Chem. 1983 submitted for publication/.

The aim of this work was to find if the influence of the above mentioned additives /2-mercaptobenzimidazole/MBIM, /phenothiazine/PT/, Permanent Red E3B/E3B/, anthracene/ANI, phenanthrene/PNR/, triphenodithiazine/TPDT/ may cause polymorphic transition retardation.

The samples were prepared during crystallization from a melt of iPP with 0.5% additive. Phase-transition from hexagonal to monoclinic form was carried out with thermal treatment in two ways: a/ step adjusted temperature in a range from 140 to 165 $^\circ$C, b/ variable time of heating /1, 2, 3, 4, 5 h./ at constant temperature close to complete transition $\beta \rightarrow \alpha$. Process of the transition, that is decrease of amount of $\beta$-form $/\beta/$, was observed on the basis of X-ray diffraction patterns.

We have found, that temperature at the initial point of rapid decrease of value of $\beta$ and the temperature at the vanishing point depend on the kind of the introduced additives.

In presence of E3B, AN, FNR, TFDT beginning of decrease was observed at definitely higher temperatures as compared to other additives. Opposite phenomenon that is faster decrease of value of $\beta$ in shorter time of thermal treatment was observed in samples with PT and MBIM. This observation corresponds to the amount of $\beta$-form found in particular samples before thermal treatment. During transition we observed increase of monoclinic form.

At the initial point of rapid decrease of amount of $\beta$-form we could see definite decrease of crystalline sizes.

The results we have obtained confirms a hypothesis of mechanism of transition and lead into conclusion that the applied additives act as retardants of polymorphic transition from hexagonal to monoclinic form. The used additives have various retardation intensity of the transition.

10.3-2 LINE GROUPS

Milan Damnjanović

Dept.of Physics, Faculty of Science, POB 550,11001 Belgrade, Yugoslavia

Line groups are symmetry groups of polymers and quasi 1-dimensional crystals. Their irreducible representations have been constructed, as well as the corresponding Clebsch-Gordan series and selection rules. For application in phase transitions studies equitranslational epikernels (low temperature subgroups) were determined. It is shown that in certain cases 3-dimensional transitions can be described by the line groups only (without reference to the space groups involved). Also, magnetic line groups and their co-representations have been derived.

References: